THE X_2BO and X_2BS (X = HYDROGEN OR HALOGEN) FREE RADICALS

DENNIS CLOUTHIER, ROBERT GRIMMINGER, BING JIN, *Department of Chemistry, University of Kentucky, Lexington, KY, USA*; PHILLIP SHERIDAN, *Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY, USA*.

The electronic spectra of the X_2BO and X_2BS free radicals have been studied by a combination of experimental and theoretical techniques. Experimentally, we have succeeded in preparing some of these species in a pulsed discharge jet and detecting them by laser-induced fluorescence and emission spectroscopy through the $\tilde{B}^2A_1 - \tilde{X}^2B_2$ transition. The radicals exhibit emission transitions down to the ground state and the low-lying $\tilde{A}^2B_1$ electronic state. We have also used high level *ab initio* theory [CCSD(T)/aug-cc-pV5Z] to calculate the properties of the ground and excited states and simulate the observed spectra. Experiment and theory agree that the radicals are planar, C_{2v} symmetry species in all the three combining states, with only small changes in geometry on electronic excitation.